X-ray Photoemission and Photoabsorption of Organic Electroluminescent Materials

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Core level and valence band photoemission as well as core level photoabsorption of thin films of Tris-(8, hydroxyquinoline) aluminum (Alq_3) and N,N'-diphenyl-N,N'-bis (3-methylphenyl)- 1,1'-biphenyl-4,4'-diamine (TPD) were studied using synchrotron radiation. Thin films of Alq_3 and TPD were sublimed from purified powders onto Si wafers in ultra high vacuum. Photoemission data were obtained with the ellipsoidal mirror analyzer (EMA) at beamline 8.0 at the Advanced Light Source while the absorption data were taken at beamline 8.2 at the Stanford Synchrotron Radiation Laboratory. Both spectroscopies were used to elucidate the element-specific electronic structure of Alq_3 and TPD. These molecules are materials of choice for organic light emitting devices (OLEDs) used in future applications such as flat panel displays [1]. For Alq_3, the experimental data were compared to calculations based on density functional theory (fig. 1). Since the calculations for the occupied density of states reproduce the measured valence band photoemission data quite well, we were able to assign all features to specific atoms/bonds in the molecule [2]. Determining the positions of the highest occupied and lowest unoccupied molecular orbitals we estimated the potential barriers at the Alq_3/TPD interface to get a better understanding of the charge transport properties of the OLED [3].

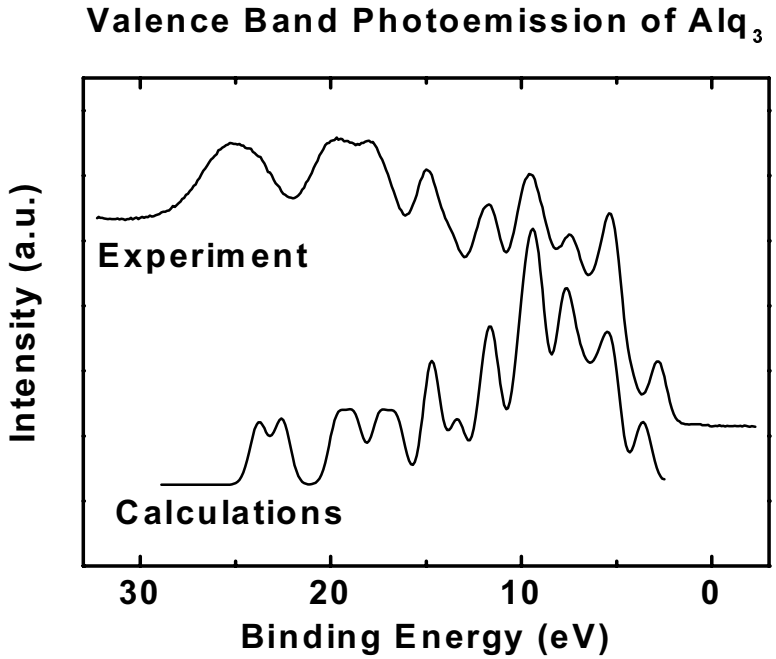

Figure 1. Comparison of the valence band photoemission of Alq_3 ($h\nu$ = 240 eV) with calculations based on density functional theory [2]. The calculations were broadened with a Gaussian function of 1.2 eV (FWHM) to account for solid state effects and experimental resolution. The good agreement between experiment and theory makes it possible to assign all features to specific atoms/bonds in the molecule [2].

A comparison of freshly evaporated films of Alq_3 and TPD with films that have been exposed to intense radiation or oxidative conditions shed light on possible damage mechanisms of the molecules [3]. This knowledge is crucial to understand and overcome present lifetime limitations of the OLEDs where oxidation and other effects lead to a significant degradation of the brightness within several 100 to a few 1000 hours. The experimental results in combination with the theoretical understanding open the way to analyze and improve the device performance, and, in particular, to tailor molecules for specific needs.

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